ATION DISCLOSURE CITATION ATTY. DOCKET NO. PC9980A SERIAL NO. 09/876,767 Use several sheets if necessary) APPLICANT M. Uchiyama, et al. **GROUP** 1631 FILING DATE June 7, 2001 **U.S. PATENT DOCUMENTS** NAME CLASS SUBCLASS FILING DATE EXAMINER INITIAL DOCUMENT NUMBER DATE **FOREIGN PATENT DOCUMENTS** DOCUMENT NUMBER DATE COUNTRY CLASS SURCI ASS LATION YES NO wo 7 19.02.98 G06F 17/50 9 8 0 0 7 International 0 6 04.05.00 International G01N OTHER DOCUMENTS (Including Author, Title, Date, Pertinent Pages, Etc.) Lien, E. J. et al., Acta Pharm. Jugosl., Vol. 34, pp. 123-131, 1984, "QSAR Analysis of the Pharmacokinetics and Metabolism of Barbiturates". Baamhielm, C. et al., Chem. Biol. Interactions, Vol. 58, pp. 277-288, 1986, "Quantitative Relationships Between Structure and Microsomal Oxidation Rate of 14-Dihydropyridines". Markin, R. S., et al., Pharmaceutical Research, Vol. 5, No.4, 1988, "Quantitative Structure-Activity Study on Human Pharmacokinetic Parameters of Benzodiazepines Using the Graph Theoretical Approach". Garcia-March, F. J., et al., J. Pharm. Pharmacol., Vol. 47, pp. 232236, 1995, "Correlation of Pharmacological Properties of a Group of β-Blocker Agents by Molecular Topology". Lombardo, F. et al., J. Med. Chem, Vol. 39, pp. 4750-4755, 1996, "Computation of Brain-Blood Partitioning of Organic Solutes via Free Energy Calculations". Palm, K. et al., J. Med. Chem, Vol. 41, pp. 5382-5392, 1998, "Evaluation of Dynamic Polar Molecular Surface Area as Predictor of Drug Absorption: Comparison with Other Computational and Experimental Predictors". Clark, D. E., Journal of Pharmaceutical Sciences, Vol. 88, No. 8, pp. 815821, August 1999, "Rapid Calculation of Polar Molecular Surface Area and Its Application to the Prediction of Transport Phenomena. 2. Prediction of BloodBrain Barrier Penetration". van de Waterbeemd, H., et al., Quant. Struct-Act. Relat. Vol. 15, pp. 480-490, 1996, "Estimation of Caco-2 Cell Permeability Using Calculated Molecular Descriptors". Kato, R. et al. English Translation of Japanese Article: Mechanisms of Drug Metabolism and Changes in Efficacy and Toxicity, Tokyo-Kagaku-Dojin, Tokyo, chapter 4, 93-123 (1995) Bush, B. L., et al., Journal of ComputerAided Molecular Design, Vol. 7, pp. 587-619, 1993, "SampleDistance Partial Least Squares: PLS Optimized for Many Variables, With Application to CoMFA". Yee, S., Pharmaceutical Research, Vol. 14, No. 6, pp. 763-766 1997, "In Vitro Permeability Across Caco-2 Cells (Colonic) Can Predict In Vivo (Small Intestinal) Absorption in Man-Fact or Myth.". **EXAMINER** DATE CONSIDERED Shit I

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